

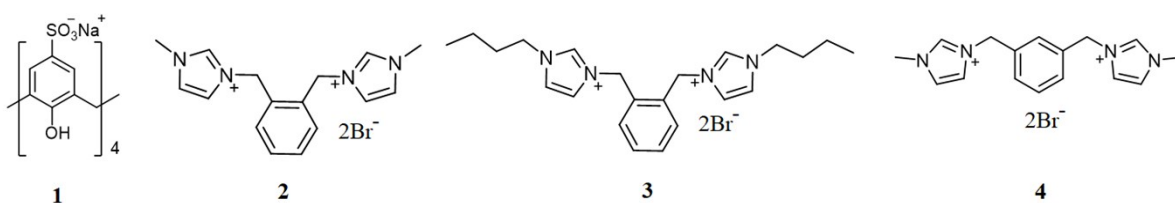
## Influence of ortho- and meta-substituted N-heterocyclic dications towards the self-assembly of *p*-sulfonatocalix[4]arene

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### Supplementary Information

Table S1: Summary of successful and unsuccessful multi-component synthesis using combinatorial approach.

Complex	1	2	3	4	PPh <sub>4</sub> <sup>+</sup> Br <sup>-</sup>	CeCl <sub>3</sub> ·7H <sub>2</sub> O	ErCl <sub>3</sub> ·6H <sub>2</sub> O	GdCl <sub>3</sub> ·6H <sub>2</sub> O
Complex I	√	√						√
Complex II	√		√			√		
Complex III	√		√				√	
Complex IV	√			√		√		
Complex V	√			√		√		
Complex VI	√			√				√
Complex VII	√			√			√	
Complex VIII	√			√	√	√		
Complex IX	√			√	√			√
Unsuccessful	√		√					√
	√		√				√	
	√			√	√			√
	√			√	√		√	
	√	√					√	
	√	√			√	√		
	√	√			√			√
	√	√					√	



1: *p*-sulfonatocalix[4]arene

2: 3,3'-(1,2-phenylenebis(methylene))bis(1-methyl-1H-imidazol-3-ium)

3: 3,3'-(1,2-phenylenebis(methylene))bis(1-butyl-1H-imidazol-3-ium)

4: 3,3'-(1,3-phenylenebis(methylene))bis(1-methyl-1H-imidazol-3-ium)

Table S2: Dihedral angles of *p*-sulfonatocalix[4]arene for complex **I** to **IX**.

<b>Complex</b>	<b>Ring 1</b>	<b>Ring 2</b>	<b>Ring 3</b>	<b>Ring 4</b>
<b>I</b>	59.19°	57.97°	57.55°	63.46°
<b>II</b>	51.00°	64.64°	39.72°	69.89°
<b>III</b>	58.44°	52.02°	64.85°	53.30°
<b>IV</b>	51.37°	67.15°	39.35°	65.03°
<b>V</b>	64.64°	44.64°	60.80°	52.46°
<b>VI</b>	48.34°	72.59°	39.64°	69.03°
<b>VII</b>	48.02°	73.08°	41.79°	70.49°
<b>VIII</b>	46.90°	72.10°	39.96°	69.74°